

Abstract Submitted
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Recent Advances in Modeling Transition Metal Oxides for Photo-electrochemistry¹ MAYTAL CASPARY TOROKER, Department of Materials Science and Engineering, Technion - Israel Institute of Technology — Computational research offers a wide range of opportunities for materials science and engineering, especially in the energy arena where there is a need for understanding how material composition and structure control energy conversion, and for designing materials that could improve conversion efficiency. Potential inexpensive materials for energy conversion devices are metal oxides. However, their conversion efficiency is limited by at least one of several factors: a too large band gap for efficiently absorbing solar energy, similar conduction and valence band edge characters that may lead to unfavorably high electron-hole recombination rates, a valence band edge that is not positioned well for oxidizing water, low stability, low electronic conductivity, and low surface reactivity. I will show how we model metal oxides with ab-initio methods, primarily DFT+U. Our previous results show that doping with lithium, sodium, or hydrogen could improve iron (II) oxide's electronic properties, and alloying with zinc or nickel could improve iron (II) oxide's optical properties. Furthermore, doping nickel (II) oxide with lithium could improve several key properties including solar energy absorption. In this talk I will highlight new results on our understanding of the mechanism of iron (III) oxide's surface reactivity. Our theoretical insights bring us a step closer towards understanding how to design better materials for photo-electrochemistry. References: 1. O. Neufeld and M. Caspary Toroker, "Pt-doped Fe₂O₃ for enhanced water splitting efficiency: a DFT+U study", J. Phys. Chem. C 119, 5836 (2015). 2. M. Caspary Toroker, "Theoretical Insights into the Mechanism of Water Oxidation on Non-stoichiometric and Ti - doped Fe₂O₃(0001)", J. Phys. Chem. C, 118, 23162 (2014).

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